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M.C. Etter, and K.S. Huang

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The Cambridge Crystallographic Data Base (CCDB) was searched for all examples of small molecules with nitroaniline groups. This data set was divided into primary and secondary nitroanilines (32 compounds), tertiary nitroanilines (36 compounds). For each set we determined what percent of the crystal structures were acentric. For the primary and secondary nitroanilines, which can form nitroaniline hydrogen bonds, 41% of the crystals were acentric. For the tertiary nitroanilines, without -NH_2---O_2N hydrogen bonds, 17% were acentric. These numbers are to be compared to the frequency of occurrence of acentricity in the CCDB for the total population of all organic molecules. This number was determined several years ago when the data base contained about 40,000 structures. At that time 25% of the structures were acentric. Within that set it is estimated that most of the acentric structures contain resolved chiral compounds. Thus, a better, yet generous, estimate for our purposes would be that only about 10% of all racemic or achiral compounds pack in acentric crystal structures. Thus, there appears to be a significant bias towards crystallographic acentricity for the primary and secondary nitroaniline structures. Further work is in progress to determine if the hydrogen-bond patterns in the primary and secondary nitroaniline class are themselves acentric.

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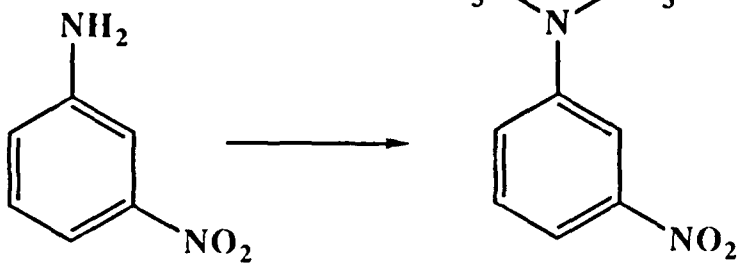
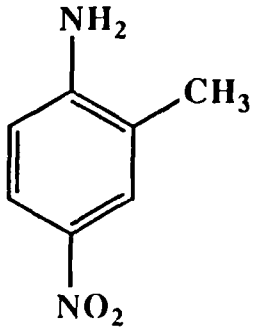
Examples of Acentric Primary Nitroanilines and Centric Tertiary Analogs

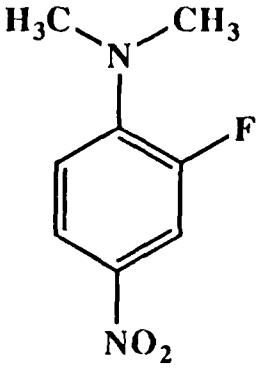


$Pbc2_1$
Acentric

$P2_1/c$
Centric



Ia
Acentric



C2/c
Centric

Both acentric compounds pack with acentric hydrogen-bond networks which may be biasing the final crystal structures to be acentric. Dipole-dipole interactions will be a less important contributor to the final packing pattern in structures with hydrogen-bonded networks than in structures without, so acentricity may be seen more frequently.

Our results show that for primary and secondary nitroanilines, acentric crystal structures occur about 40% of the time, while for tertiary nitroanilines acentricity occurs 17% of the time (about the same rate as for other achiral molecules).